Pestic. Sci. 1997, **49**, 210–212

Extended Summary SCI Pesticides Group Meeting Ecotoxicology of Organic Compounds in the Aquatic Environment

The following is an extended summary based on a paper presented at the meeting 'Ecotoxicology of Organic Compounds in the Aquatic Environment', organised by P. Nicholls and R. Greenwood on behalf of the Physicochemical and Biophysical Panel of the SCI Pesticides Group and held on 5 December 1995 at 14/15 Belgrave Square, London. It is entirely the responsibility of the author and does not necessarily reflect the views of the Editorial Board of Pesticide Science.

Exposure Assessment of Pesticides in Field Ditches: the TOXSWA Model

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1 *Introduction*

Application of pesticides to agricultural fields may result in their entry into surface waters. Many agricultural fields in the Netherlands are surrounded by field ditches, which drain excess water or which are used to infiltrate water into the fields or to prevent the rapid lowering of the water table in the summer season. In pesticide approval procedures, the risks of pesticides to aquatic organisms are commonly assessed by comparing estimated exposure concentrations in the field with laboratory toxicity data on some standard test organisms (algae; Daphnia; fish). We developed the TOXSWA computer model (TOXic substances in Surface WAters) to estimate short- and long-term exposure in field ditches. The model will be used in the Dutch pesticide approval procedure in the near future.[1]

The TOXSWA model describes the fate of pesticides entering field ditches (i) by drift or atmospheric deposition, (ii) by surface runoff or (iii) by drainage or leaching through the soil. Entries in the simulated system can be instantaneous or distributed over a certain period. The entries can emanate from a point or be distributed over a certain length of ditch.

2 *Field ditch system and processes*

Figure 1 shows an outline of the modelled ditch. Its geometry as well as the flow velocity and the water depth can be freely chosen and it is assumed that the field ditch permanently carries water. As shown by Fig. 1, the simulated field ditch is two-dimensional and consists of a water layer containing suspended solids and macrophytes, and a sediment layer whose properties (porosity, organic matter content and bulk density) vary with depth. The vertical cross-section of the ditch has a trapezoidal shape. In the water layer, the pesticide concentration is assumed to be constant in the vertical direction, but varies in the horizontal direction. In the sediment layer, the pesticide concentration is a function in both the horizontal and vertical directions.

TOXSWA considers four processes: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilisation (Fig. 1). In the water layer, pesticides are transported by advection and dispersion, whereas, in the sediment, diffusion is included as well. The transformation rate covers the combined effects of hydrolysis, photolysis and biodegradation; metabolites are not considered.

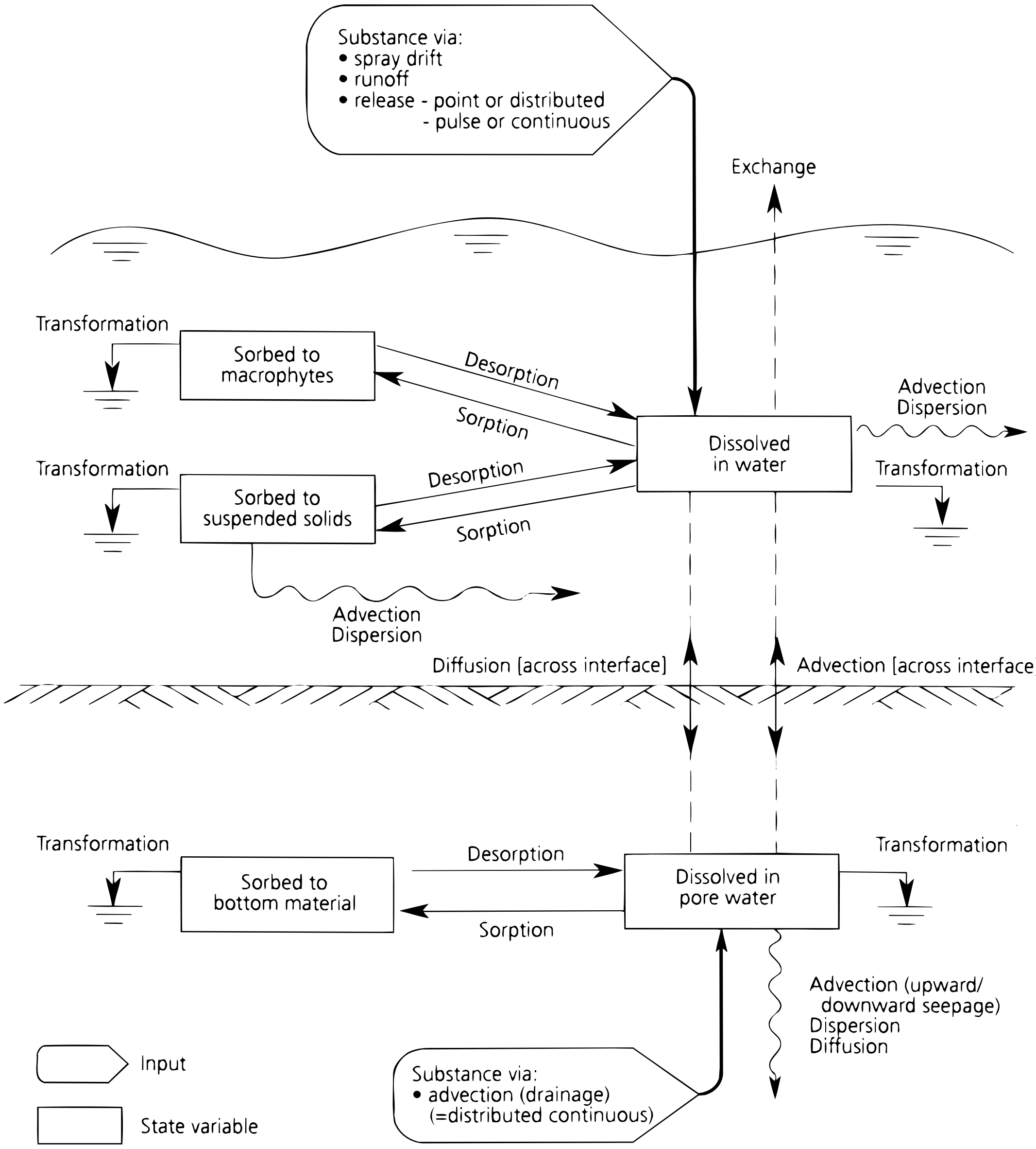

Fig. 1. Diagram of modelled field ditch.

Sorption to suspended solids and to sediment is described by the Freundlich equation. Sorption to macrophytes is described by a linear isotherm. Pesticides are transported across the water–sediment interface by advection (upward or downward seepage) and by diffusion.

Mass balances for an elemental volume in the water layer and in the sediment link all the processes together; the mass balances result in two differential equations which are solved using a generalised finite-difference method. For the numerical solution, the water layer is divided into a number of nodes in the horizontal direction. Below each node, a number of nodes are defined for the sediment layer. Distances between the nodes in the water and sediment layers are of the order of metres and millimetres, respectively. The numerical solution is implemented as the TOXSWA computer program. Finally, it is verified that the computer program adequately represents the mathematical model, i.e. the mass balances. For example, it has been checked that the mass of pesticide introduced (100%) can be traced at every moment with an error of less than 0·1%.

3 *Sample simulations*

To illustrate the use of the model, a calculation was carried out for a moderately sorbing, hypothetical pesticide (K_{om} ‡ of 250 litres kg^{-1}) (Table 1). The water flow

‡ K_{om} is defined as the slope of the sorption isotherm of suspended solids or of sediment material, based on the organic matter content (litres kg^{-1}).

TABLE 1
Overview of inputs into the model for the sample simulation

Ditch characteristics:	
Length of field ditch:	200 m
Water flow rate:	100 m day^{-1}
Water depth:	0·50 m
Side slope (hor/vert):	2
Density of macrophytes:	250 g m^{-2}
Concentration of suspended solids:	50 g m^{-3}
Sediment characteristics:	
Thickness:	0·10 m
Porosity:	0·4–0·8
Organic matter content:	0·5–8%
Pesticide characteristics:	
Half-life due to transformation in water:	100 days
Half-life due to transformation in sediment:	75 days
Slope of sorption isotherm for macrophytes:	2000 litres kg^{-1}
Slope of sorption isotherm for suspended solids:	25 litres kg^{-1}
Slope of sorption isotherm for sediment on organic matter basis (K_{om}):	250 litres kg^{-1}

rate was 100 m day^{-1} and there was no seepage through the sediment. A single pesticide entry by spray drift (3% of an application rate of 1 kg ha^{-1}) was simulated, occurring over the total length of the ditch, except for the first 20 m. Initially, the sediment was free of pesticide. Immediately after application, 56% of the applied mass was dissolved in the ditch water and 44% was adsorbed to the macrophytes. After one day, 54% of the pesticide mass in the total ditch was dissolved in the water, 43% was sorbed to the macrophytes, 0·1% was sorbed to the suspended solids and 2·3% was present in the sediment. A total concentration of about ten times the water concentration built up in the sediment, with a penetration depth of about 5 mm. Next, the concentration front moved out of the ditch and back-diffusion of residues from the sediment into the water layer started. After four days, the water, macrophyte and sediment compartments each contained about one-third of the total pesticide mass present.

4 *Future projects*

The first version of the TOXSWA model was released in April 1996, including a theoretical description and a user's manual.[2,3] Improvements to the model are planned in two areas: (i) inclusion of multiple or continuous pesticide applications to the water and (ii) implementation of time series with varying water flow rates and water depths. Model validation will start, firstly, by using data sets from four experiments performed at the DLO Winand Staring Centre.[4] Subsequently, the sensitivity of the model will be analysed. Finally, standard scenarios for the Netherlands will be defined to facilitate the use of the model for risk assessments in the Dutch pesticide approval procedure. A study of the sorption of a range of pesticides to three plant species is being carried out, because very little information is available on this sorption parameter.

Acknowledgements

The author wishes to thank Dr Theo C. M. Brock and Dr Jos J. T. I. Boesten of the DLO Winand Staring Centre for their useful comments on the manuscript. The research was part of the Multi-Year Crop Protection Plan of the Dutch Government.

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